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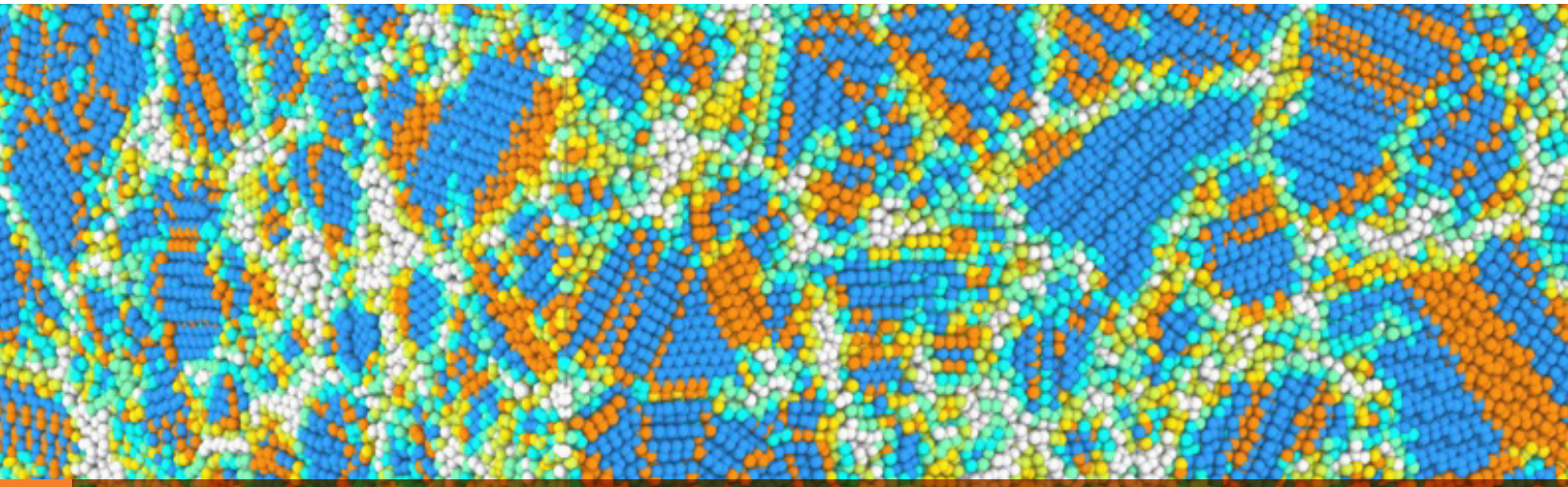

MACHINE LEARNING REVEALS WATER'S COMPLEX PROPERTIES

THE IMPETUS

While water is perceived to be one of the simplest substances in the world, modeling its behavior on the atomic or molecular level has frustrated scientists for decades. To date, no single model has been able to accurately represent the plethora of water's singular characteristics, including the fact that it is densest at a temperature slightly higher than its melting point.

Researchers at the Center for Nanoscale Materials (CNM), a U.S. Department of Energy (DOE) Office of Science user facility located at Argonne National Laboratory, together with CNM users from Argonne, the University of Louisville and the University of Chicago, achieved a breakthrough in the effort to mathematically represent how water behaves. To do so, the team used machine learning to develop a new, computationally inexpensive water model that more accurately represents the thermodynamic properties of water, including how water changes to ice at the molecular scale.

THE WORK

Trying to create quantum mechanical or atomistic models to capture water's behavior had flummoxed researchers because they are so computationally intensive and still fail to reproduce many temperature-dependent properties of water.

The team used the high-performance computing resources of the Carbon cluster at CNM, the Mira supercomputer at the Argonne Leadership Computing Facility, a DOE Office of Science user facility, Fusion at Argonne's Laboratory Computing Resource Center, and the National Energy Research Scientific Computing Center, to perform simulations of up to 8 million water molecules to study the growth and formation of interfaces in polycrystalline ice.

To achieve the high accuracy of the coarse-grained model, the researchers trained the model using information drawn from nearly a billion atomic-scale configurations involving temperature-dependent properties that are well known.

THE IMPACT

This new model, termed "coarse-grained," achieves a fidelity on par with models that incorporate an atomic-level description. For the researchers, the choice to use entire water molecules as the fundamental unit in the model allowed them to perform the simulation at low computational cost. The researchers also showed that their approach could be used to improve the performance of other existing atomistic and molecular models.

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